Electronic Absorption, Emission and Two-Photon Absorption Properties of Some Extended 2,4,6-Triphenyl-1,3,5-triazines

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Including:

1. Synthesis and characterization of known compounds

2,4,6-tris(4-bromophenyl)-1,3,5-triazine (8-Br).[1] A flask containing triflic acid (9 mL, 15 g, 102 mmol) under argon was cooled to 0-4 °C (ice bath). In batches of approximately 0.5 g solid 4-bromobenzonitrile (4.67 g, 25.6 mmol) was added with stirring, the addition takes about 1.5 h. The homogenous, yellow solution was allowed to slowly warm to room temperature and stirred overnight. The reaction was quenched with ice and then neutralized using aqueous NH_4OH solution. The white precipitate was collected on a glass frit and thoroughly washed with water (3 × 10 mL) followed by acetone (2 × 10 mL) and acetone/dichloromethane (1:1 mixture, 2 × 10 mL). The solid was air-dried for 2 h then transferred to flask and dried under high vacuum for 6 h giving the title compound as a white powder (4.34 g, 7.9 mol, 93%). Spectroscopic characterisation matched that reported in the literature.[2] **^{1}H NMR (300 MHz, $CDCl_3$):** δ = 8.62 (m, 2H, AA′XXэ, H_{Ph}); 7.73 (m, 2H, AA′XX′, H_{Ph}). **IR (KBr, cm^{-1}):** ῡ = 3060, 3035 (vw, C_{Ar}-H); 1580 (s); 1512 (overlapping, C=C_{Ar}/C=$N_{triazine}$, s). **Raman (neat, cm^{-1}):** ῡ = 1590 (vs, C=C_{Ar}); 1580 (w, sh); 1513 (m, C=$N_{triazine}$); 989 (s, C=$N_{triazine}$).

2,4,6-tris(4-iodophenyl)-1,3,5-triazine (8-I). In a round bottom flask under argon, triflic acid (5 ml) was cooled to 0-4 °C (ice bath). Solid 4-iodobenzonitrile (2.33 g) was added in batches, with stirring, over a period of 1 h. The homogenous, yellow solution was allowed to slowly warm to room temperature and stirred overnight. The reaction mixture was quenched with ice and then neutralized with aqueous NH_4OH solution. The white precipitate was collected on a glass frit and washed with water (3 × 10 mL), acetone (2 × 10 mL) and finally acetone/CH_2Cl_2 (1:1 mixture, 2 × 10 mL). The solid was air dried for 1 h then transferred to a flask and dried under high vacuum for 8 h. The title compound was isolated a white powder (1.98 g, 85%). **HRMS (ASAP):** m/z = 687.8240 $[M+H]^+$ (calc. for $C_{21}H_{13}N_3I_3$: 687.8244). **Anal. Calc. for $C_{21}H_{12}N_3I_3$:** C, 36.71, H, 1.76, N, 6.12; found: C, 36.52, H, 1.76, N, 6.15. Spectroscopic characterisation matched that reported in the literature.[2] **^{1}H NMR (300 MHz, $CDCl_3$):** δ = 8.44 (m, 2H, AA′XX′, H_{Ph}); 7.93 (m, 2H, AA′XX′, H_{Ph}). **IR (KBr, cm^{-1}):** ῡ = 3060 and 3035 (vw, C_{Ar}-H); 1576 (s, C=C_{Ar}); 1525-1506 (overlapping, vs, C=C_{Ar}/C=$N_{triazine}$). **Raman (neat, cm^{-1}):** ῡ = 3064 (w, C_{Ar}-H); 1590 (vs, C=C_{Ar}); 1527-1508 (overlapping, m, C=C_{Ar}/C=$N_{triazine}$); 990 (m, C=$N_{triazine}$).

2,4,6-tris{4-(2-trimethylsilylethynyl)phenyl}-1,3,5-triazine (8-C≡CTMS). This compound was obtained following a modification of the literature procedure reported by Jia and coworkers.[3] An oven-dried Schlenk flask was charged with **8-Br** (501 mg, 0.917 mml), $Pd(PPh_3)_4$ (63 mg, 0.054 mmol) and CuI (22 mg, 0.115 mmol) and degassed (4 × vacuum/argon cycles). Degassed NEt_3 (15 mL) was added using a cannula transfer followed by ethynyl trimethylsilane (0.7 mL, 4.9 mmol). The flask was

fitted with a condenser and the reaction mixture refluxed for 2 days. The mixture was allowed to cool slightly then filtered to the remove the insoluble salts, the solid was washed with hot NEt_3. The filtrate was allowed to cool to room temperature and then placed in a fridge for 3 h, the white precipitate was collected on a glass frit and washed with hexanes. The solid was recrystallized from hot hexanes and dried under reduced pressure (high vacuum, 6 h) giving the title product as fluffy, colourless needles (330 mg, 60%). **MP:** 268 °C. **HRMS (ASAP):** m/z = 598.2527 $[M+H]^+$ (calc. for $C_{36}H_{40}N_3Si_3$: 598.2530). Spectroscopic characterisation matched these reported in the literature.[3, 4] **^{1}H NMR (300 MHz, $CDCl_3$):** δ = 8.69 (m, 6H, AA'XX', H_{Ph}); 7.65 (m, 6H, AA'XX' H_{Ph}); 0.30 (s, 27H, SiCH_3). **IR (KBr, cm^{-1}):** $\bar{\upsilon}$ = 2958 (m, C_{Ar}-H), 2898 (w, C_{Ar}-H), 2157 (s, C≡C), 1604 (m), 1572 (s), 1511 (vs, C=$N_{triazine}$). **Raman (neat, cm^{-1}):** $\bar{\upsilon}$ = 2960 (m, C_{Ar}-H); 2900 (w, C_{Ar}-H); 2160 (s, C≡C); 1604 (vs, C=C_{Ar}); 1513 (m, C=$N_{triazine}$); 991 (w, C=$N_{triazine}$). **UV-Vis (CH_2Cl_2, nm [ε, 10^3 M^{-1}cm^{-1}]):** λ_{max} = 320 [106].

2,4,6-tris(4-ethynylphenyl)-1,3,5-triazine (8-C≡CH). In a round bottom flask, K_2CO_3 (5.37 g) was added to a solution of **8-C≡CTMS** (125 mg, 0.209 mmol) in methanol/CH_2Cl_2/H_2O (15 mL / 50 mL / 1.5 mL). The mixture was stirred at room temperature for 2 h then filtered. The solid was thoroughly washed with CH_2Cl_2 and then the filtrate was concentrated under reduced pressure (rotavap). The resulting precipitate was collected on a glass frit, washed with methanol and dried giving the title compound as a colourless powder (55 mg, 69%). **HRMS (ASAP):** m/z = 381.128 $[M+H]^+$ (calc. for $C_{27}H_{16}N_3$: 381.127). Spectroscopic characterisation matched these reported in the literature.[3, 4] **^{1}H NMR (300 MHz, $CDCl_3$):** δ = 8.72 (d, *J* = 8.4 Hz, AA'XX', 6H, H_{Ph}, H2'/6'); 7.69 (d, *J* = 8.4 Hz, AA'XX', 6H, H_{Ph}, H3'/5'); 3.28 (s, 3H, C≡CH). **IR (KBr, cm^{-1}):** $\bar{\upsilon}$ = 3287, 3238 (m, s, C_{Ar}-H & ≡C-H); 1605 (w, C=C_{Ar}); 1574 (s, C=C_{Ar}); 1514 (vs, C=$N_{triazine}$). **Raman (neat, cm^{-1}):** $\bar{\upsilon}$ = 2110 (s, C≡C); 1605 (vs, C=C_{Ar}); 1576 (vw, C=C_{Ar}); 1514 (m, C=$N_{triazine}$); 990 (w, C=$N_{triazine}$). **UV-Vis (CH_2Cl_2, nm [ε, 10^3 M^{-1}cm^{-1}]):** λ_{max} = 303 [90].

2,4,6-tris{4′-[(4′′-cyano)-2′′′-phenylethynyl]phenyl}-1,3,5-triazine (3-CN). A dry Schlenk flask was charged with **8-I** (200 mg, 0.291 mmol), $Pd(PPh_3)_4$ (34 mg, 0.029 mmol) and CuI (11 mg, 0.058 mmol) and then degassed (4 × vacuum/argon cycles). A degassed mixture of DMF/NEt_3 (3/1 mixture, 25 mL) was added using a cannula and finally ethynylbenzonitrile (185 mg, 1.45 mmol). The flask was sealed and heated at 55-60 °C for 3 days. The solvent was removed *in vacuo* and the residue dissolved in CH_2Cl_2 and washed with water (2 × 20 mL), dried ($MgSO_4$) and solvent removed under reduced pressure. The crude product was purified using flash column chromatography (Silica gel, eluting with $CHCl_3$) giving the title product as a colourless powder (70 mg, 35%). **HRMS (ASAP):** m/z = 685.2136 $[M+H]^+$ (calc. for $C_{48}H_{25}N_6$: 685.2135). **Anal. Calc. for $C_{48}H_{24}N_6 \bullet H_2O$**: C, 82.04, H, 3.73, N, 11.96; found: C, 82.11, H, 3.86, N, 11.36. Spectroscopic characterisation matched that reported in the literature.[5] **^{1}H NMR (400 MHz,**

$CDCl_3$): δ = 8.79 (d, splitting = 8.2 Hz, 6H, AA'XX', H_{Ph}); 7.75 (d, *J* = 8.2 Hz, 6H, AA'XX', H_{Ph}); 7.68 (s, 12H, $H_{Ph'}$). **$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$):** δ = 171.1 (*C*, $C_{triazine}$); 136.3 (C_{Ph}); 132.3 ($C_{Ph}H$); 132.2 ($C_{Ph}H$); 132.1 ($C_{Ph'}H$); 129.0 ($C_{Ph}H$); 127.8 ($C_{Ph'}$); 126.6 (C_{Ph}); 118.4 (*C*, CN); 112.0 (*C*, $C_{Ph'}$); 93.1 (C≡*C*); 90.5 (*C*≡C). **IR (KBr, cm^{-1}):** ῡ = 2224 (m, CN or C≡C); 1604 (m, C=C_{Ar}); 1569 (m, C=C_{Ar}); 1511 (vs, C=$N_{triazine}$). **Raman (neat, cm^{-1}):** ῡ = 2218 (s, CN or C≡C)**;** 1605 (vs, C=C_{Ar}); 1519 (w, C=$N_{triazine}$); 991 (w, C=$N_{triazine}$).

2,4,6-tris{4′-[(4′′-methoxy)-2′′′-phenylethynyl]phenyl}-1,3,5-triazine (3-OMe). A dry Schlenk flask was charged with **8-Br** (338 mg, 0.619 mmol), $Pd(PPh_3)_4$ (72 mg, 0.062 mmol) and CuI (25 mg, 0.131 mmol) then degassed (4 × vacuum/argon cycles). Degassed NEt_3 (30 mL) was added using a cannula followed by ethynyl anisole (406 mg, 3.072 mmol). The flask was sealed and heated at 70 °C for 8 h. The reaction was allowed to cool slightly and analysed by TLC, the reaction was not complete probably due to a solubility issue, so degassed THF (30 mL) was added and heating resumed for another 18 h. The reaction mixture was allowed to cool to room temperature, filtered and the solvent removed *in vacuo*. The residue was dissolved in CH_2Cl_2 and applied to a short column of silica, the plug was washed with an ethylacetate/hexanes mixture [1:5] to remove the excess starting alkyne and was then extracted with CH_2Cl_2 then with $CHCl_3$. The combined CH_2Cl_2/$CHCl_3$ solution was concentrated and hexanes added, the product precipitated and was collected on a glass frit and dried under reduced pressure. The product was isolated as a pale yellow powder (227 mg, 52%). **HRMS (ASAP):** m/z = 700.2599 $[M+H]^+$ (calc. for $C_{48}H_{34}N_3O_3$: 700.2595). **Anal. Calc. for $C_{48}H_{33}N_3O_3$:** C, 82.38, H, 4.75, N, 6.00; found: C, 81.93, H, 4.74, N, 6.01. Spectroscopic characterisation matched that reported in the literature.[6] **^1H NMR (400 MHz, $CDCl_3$):** δ = 8.74 (d, *J* = 8.0 Hz, 6H, H_{Ph}); 7.70 (d, *J* = 8.0 Hz, 6H, H_{Ph}); 7.53 (d, *J* = 8.4 Hz, 6H, $H_{Ph'}$); 6.91 (d, *J* = 8.4 Hz, 6H, $H_{Ph'}$); 3.85 (s, 9H, OCH_3). **$^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$):** δ = 171.2 ($C_{triazine}$); 160.1 (C_{Ph}'); 135.5 (C_{Ph}); 133.4 ($C_{Ph'}H$); 131.8 ($C_{Ph}H$); 129.0 ($C_{Ph}H$); 128.1 (C_{Ph}); 115.2 (C_{Ph}'); 114.3 ($C_{Ph'}H$); 92.6 (*C*≡C); 88.3 (C≡*C*); 55.5 (CH_3). **IR (KBr, cm^{-1}):** ῡ = 2833 (w, C_{Ar}-H); 2209 (m, C≡C); 1599 (s, C=C_{Ar}); 1568 (s, C=C_{Ar}); 1512 (vs, C=$N_{triazine}$). **Raman (neat, cm^{-1}):** ῡ = 2213 (s, C≡C); 1603 (vs, C=C_{Ar}); 1512(m, C=$N_{triazine}$); 990 (w, C=$N_{triazine}$).

2,4,6-tris{4′-[(4′′-diphenylamino)-2′′′-phenylethynyl]phenyl}-1,3,5-triazine (3-NPh_2). A dry Schlenk flask was charged with **8-Br** (102 mgs, 0.187 mmol), $Pd(PPh_3)_4$ (23 mg, 0.020 mmol) and CuI (7 mg, 0.037 mmol) and then degassed (4 × vacuum/argon cycles). Degassed NEt_3 (7 mL) was added using a cannula followed by degassed DMF (14 mL). The alkyne was rapidly added under a stream of argon then the flask was sealed. The reaction mixture was heated at 70 °C for 5 days. The solvent was removed *in vacuo*, the residue dissolved in CH_2Cl_2 (100 mL), washed with water (3 x 15 mL) and dried ($MgSO_4$). The solvent was removed under reduced pressure and the crude material was purified using column

chromatography (neutral alumina, 3.5 cm × 15 cm, eluting with a CH_2Cl_2/hexanes [1:5] mixture), the title compound was then precipitated from CH_2Cl_2/hexane as a bright yellow powder (123 mg, 60%). **HRMS (ESI, $CHCl_3$/MeOH[9:1]):** m/z = 1110.4402 $[M]^+$ (calc. for $C_{81}H_{54}N_6$: 1110.4404). **Anal. Calc. for $C_{81}H_{54}N_6$:** C, 87.54, H, 4.90, N, 7.56; found: C, 86.85, H, 5.02, N, 7.35. Spectroscopic characterisation matched that reported in the literature.[4] **^{1}H NMR (400 MHz, CD_2Cl_2):** δ = 8.75 (d, *J* = 8.0 Hz, 6H, H_{Ph}); 7.71 (d, *J* = 8.0 Hz, 6H, $H_{Ph'}$); 7.42 (d, *J* = 8.4 Hz, 6H, $H_{Ph'}$); 7.30 (m, 12H, H_{NPh2}); 7.14-7.07 (m, 18H, H_{NPh2}); 7.00 (d, *J* = 8.4 Hz, 6H, $H_{Ph'}$).**^{13}C{^{1}H} NMR (101 MHz, CD_2Cl_2):** δ = 171.4 ($C_{triazine}$); 148.8 ($C_{Ar}H$); 147.4 (NC_{Ph}); 135.7 (C_{Ar}); 133.0 ($C_{Ar}H$); 131.9 ($C_{Ar}H$); 129.8 (C_{NPh2}); 129.2 ($C_{Ar}H$); 128.4 (C_{Ar}); 125.6 (C_{NPh2}); 124.2 (C_{NPh2}); 122.1 ($C_{Ar}H$); 115.6 (C_{Ar}); 93.2 (C≡*C*); 88.7 (*C*≡C). **IR (KBr, cm^{-1}):** $\bar{\upsilon}$ = 3062 (w, C_{Ar}-H); 2207 (m, C≡C); 1590 (s, C=C_{Ar}); 1570 (m, C=C_{Ar}); 1506 (vs, C=$N_{triazine}$). **Raman (neat, cm^{-1}):** $\bar{\upsilon}$ = 3033 (vw, C_{Ar}-H); 2208 (s, C≡C); 1605 (vs, C=C_{Ar}); 1509 (w, C=$N_{triazine}$); 992 (w, C=$N_{triazine}$).

2. ^{1}H / $^{13}C\{^{1}H\}$ NMR spectra of selected compounds

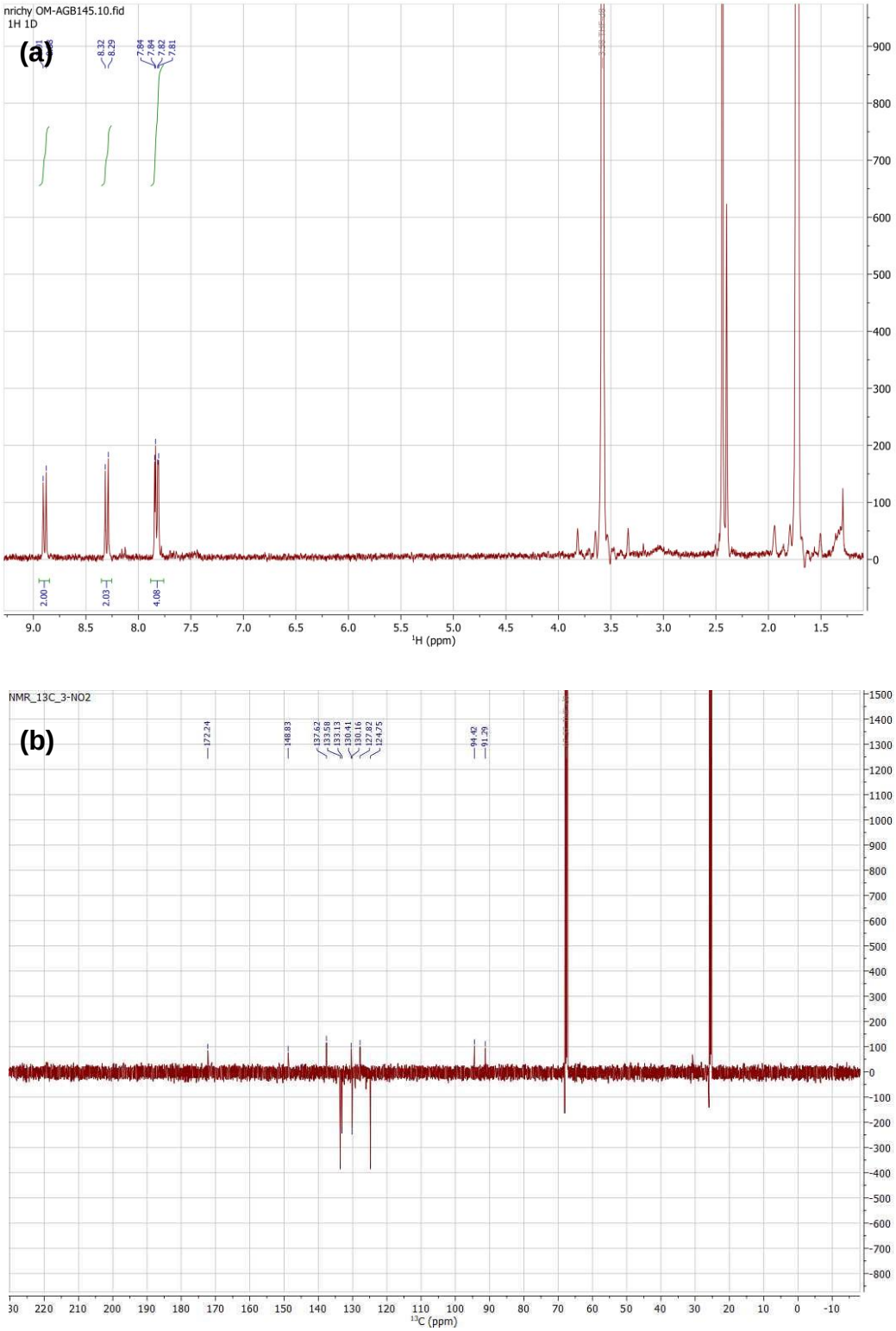


Figure S1. ^{1}H (a) and $^{13}C\{^{1}H\}$ (b) NMR spectra at 300 and 125 MHz, respectively, for **3-NO$_2$** in THF-d_8.

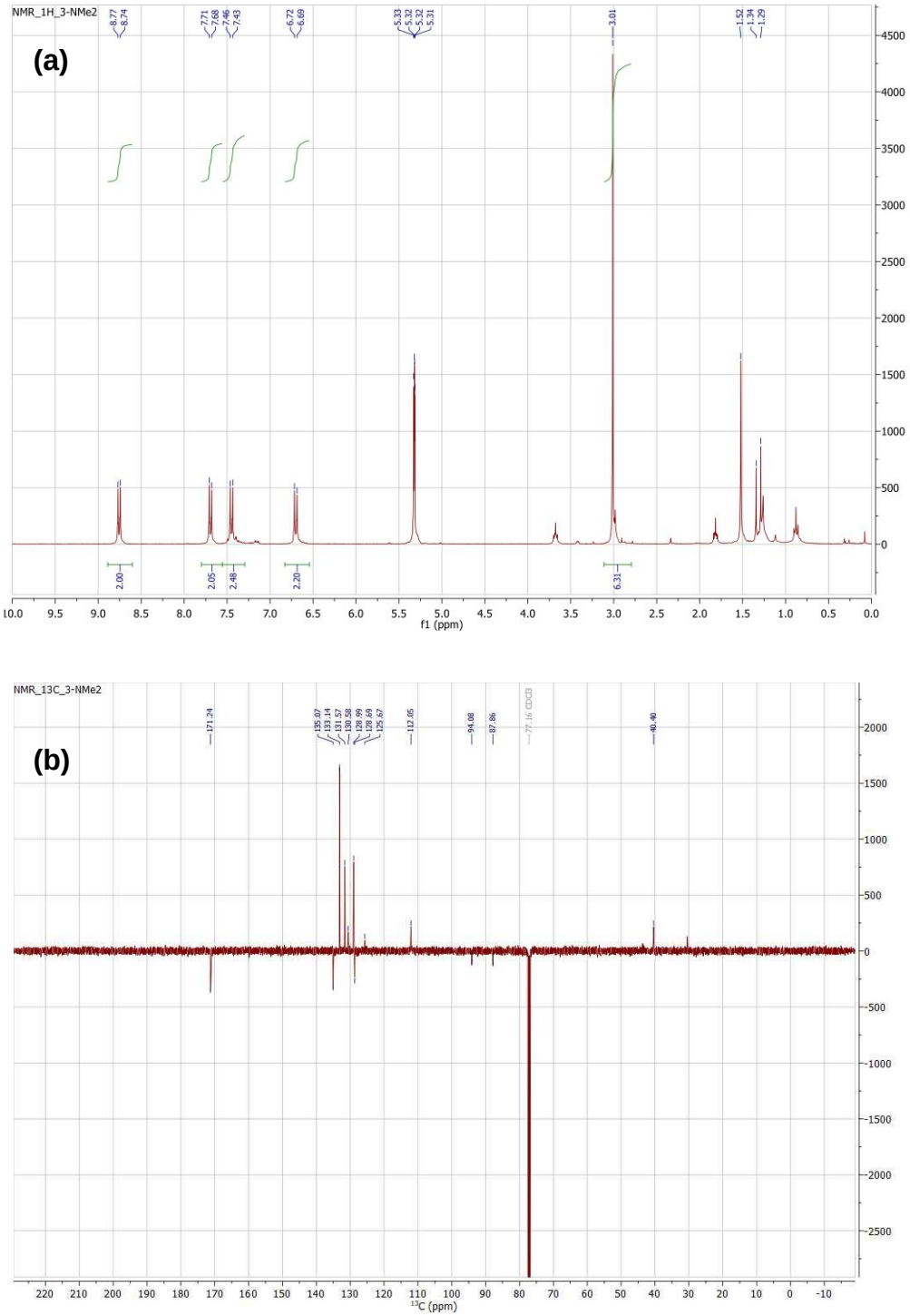


Figure S2. ^{1}H (a) and $^{13}C\{^{1}H\}$ (b) NMR spectra at 500 and 126 MHz, respectively, for **3-NMe$_2$** in CD_2Cl_2.

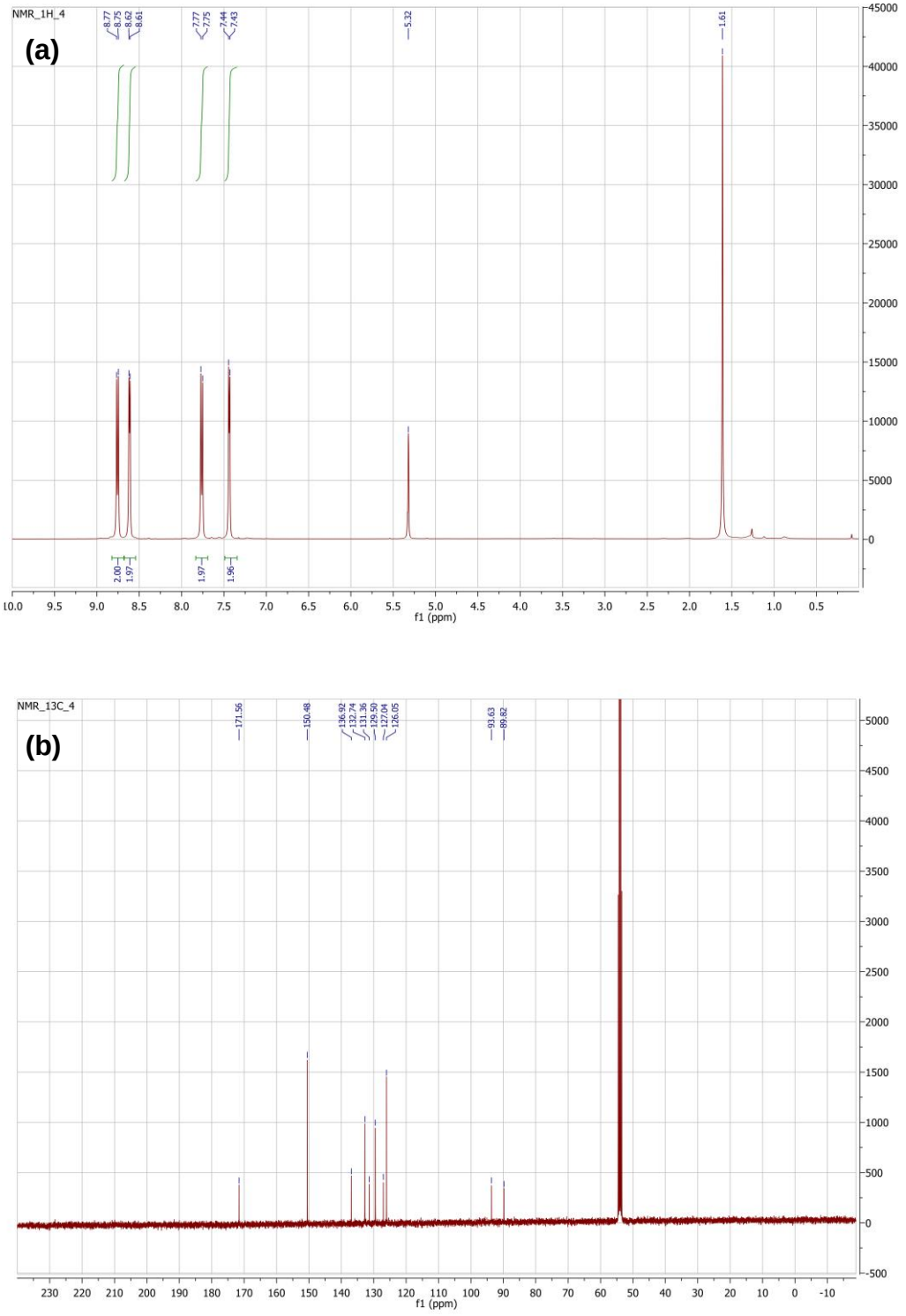


Figure S3. ^{1}H (a) and $^{13}C\{^{1}H\}$ (b) NMR spectra at 400 and 101 MHz, respectively, for **4** in CD_2Cl_2.

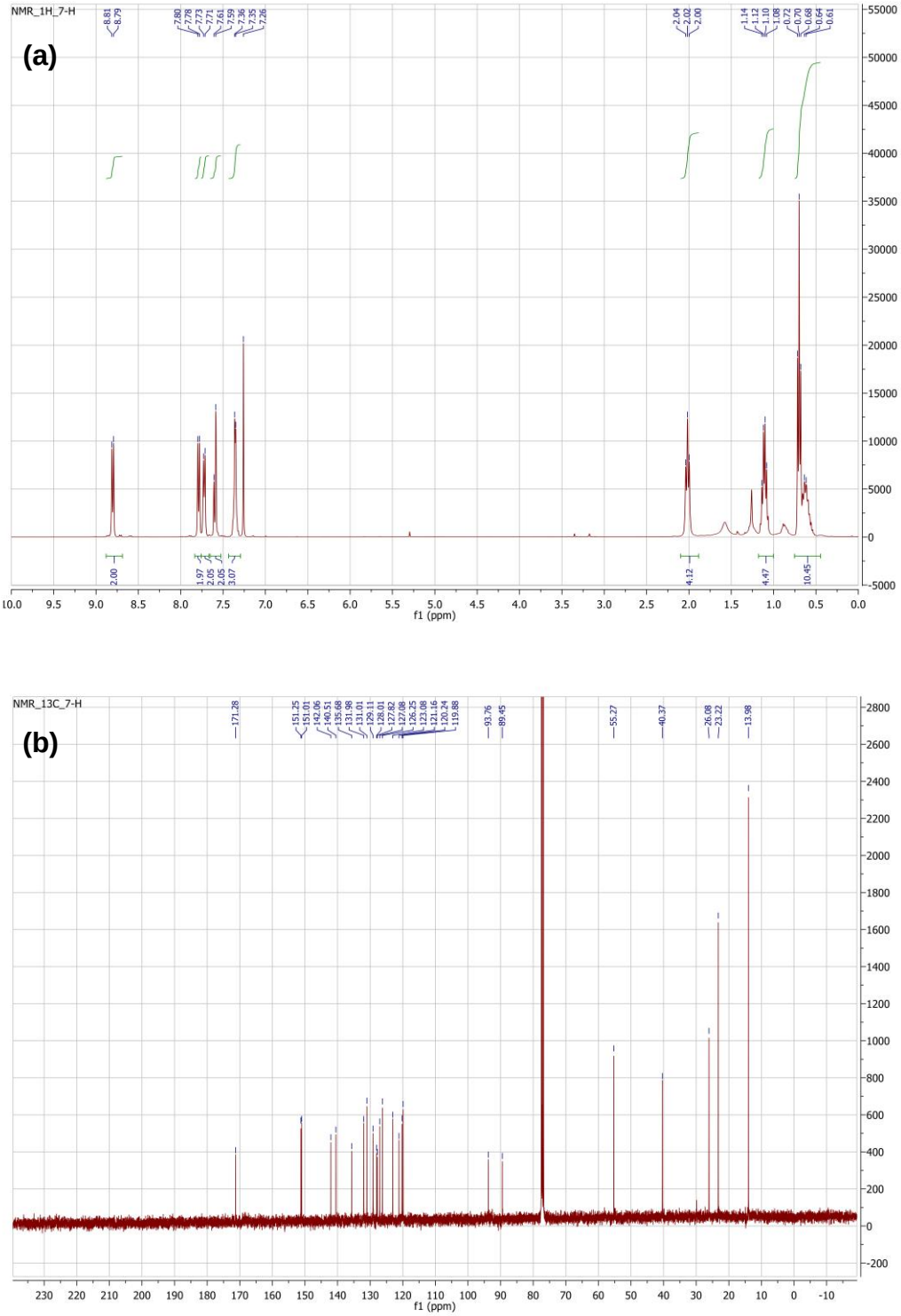


Figure S4. ^{1}H (a) and $^{13}C\{^{1}H\}$ (b) NMR spectra at 400 and 101 MHz, respectively, for **7-H** in $CDCl_3$.

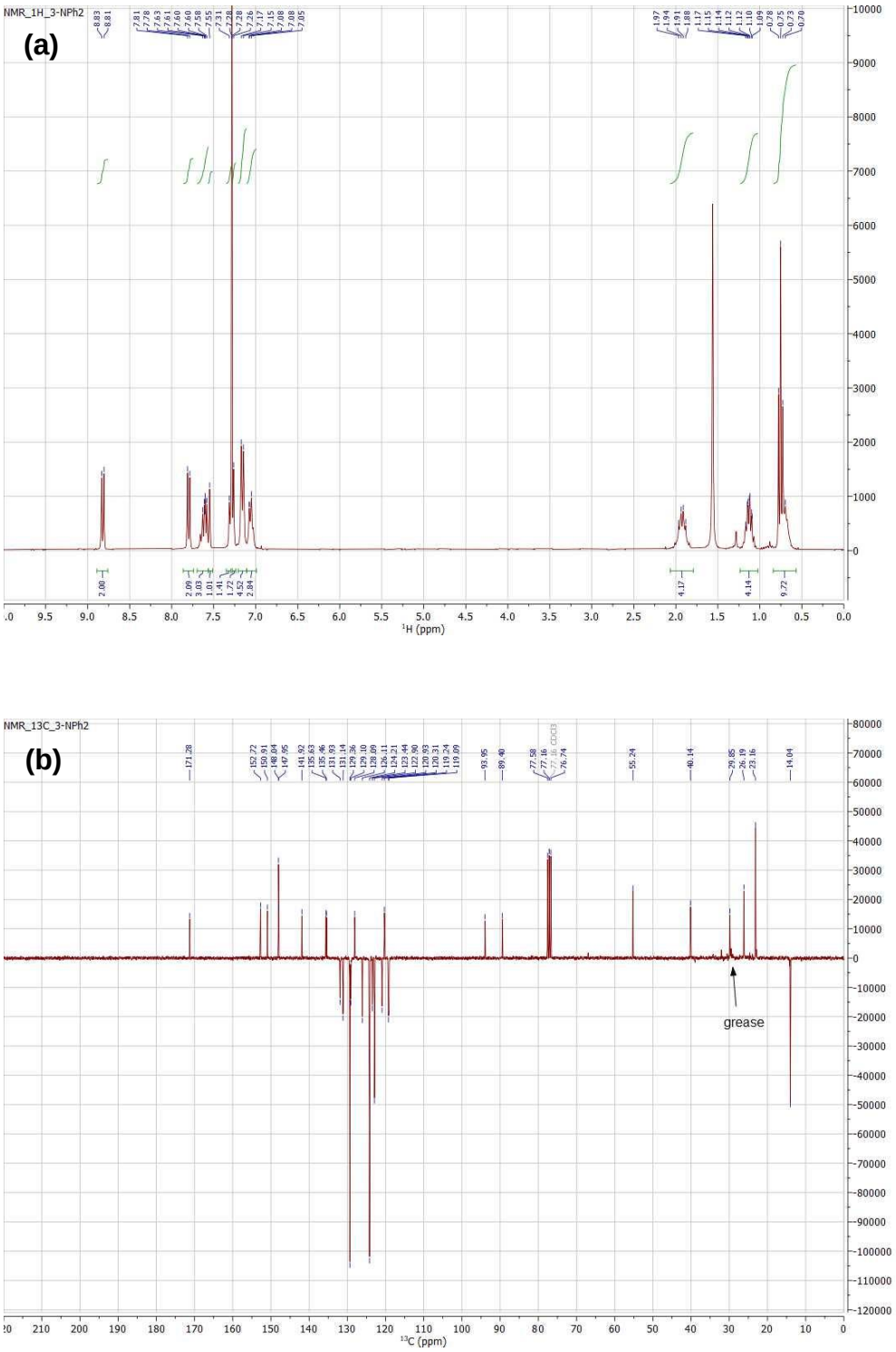


Figure S5. ^{1}H (a) and ^{13}C{^{1}H} (b) NMR spectra at 300 and 75 MHz, respectively, for **7-NPh$_2$** in $CDCl_3$.

3. Absorption/emission data for 3-X, 4 and 7-X

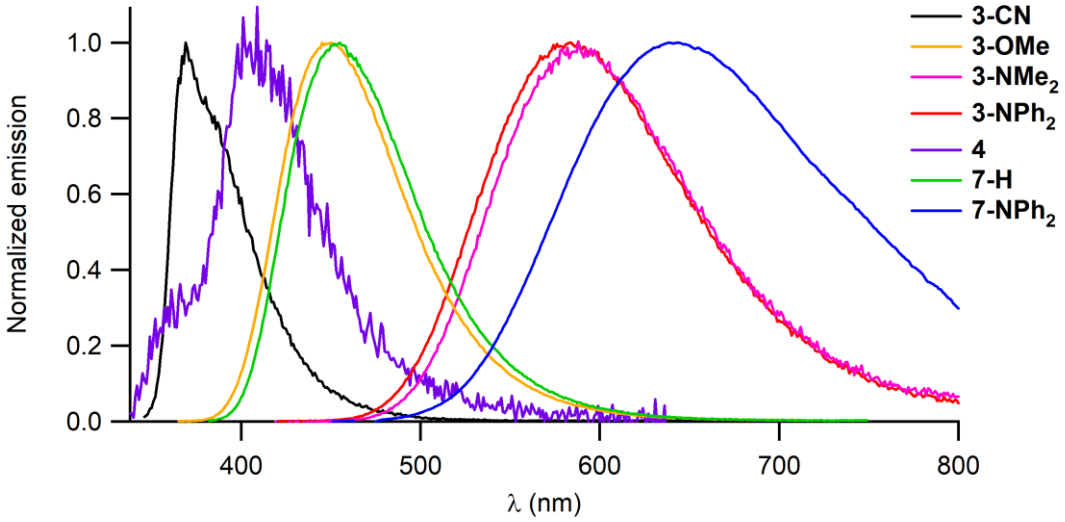


Figure S6. Emission spectra of compounds **3-X**, **4** and **7-X** in CH_2Cl_2 at 298K.

Table S1. Absorption and emission properties of **3-NO₂**, **3-NPh₂** and **7-H** in THF at 25 °C.

Cmpd	λ_1 (max) [nm]	λ_{em} [nm]	Φ_F[a]	Stokes shift [cm^{-1}]
3-NO₂	348	554	0.05	10685
3-NPh₂	405	568	0.73	7086
7-H	376	440	0.78	3658

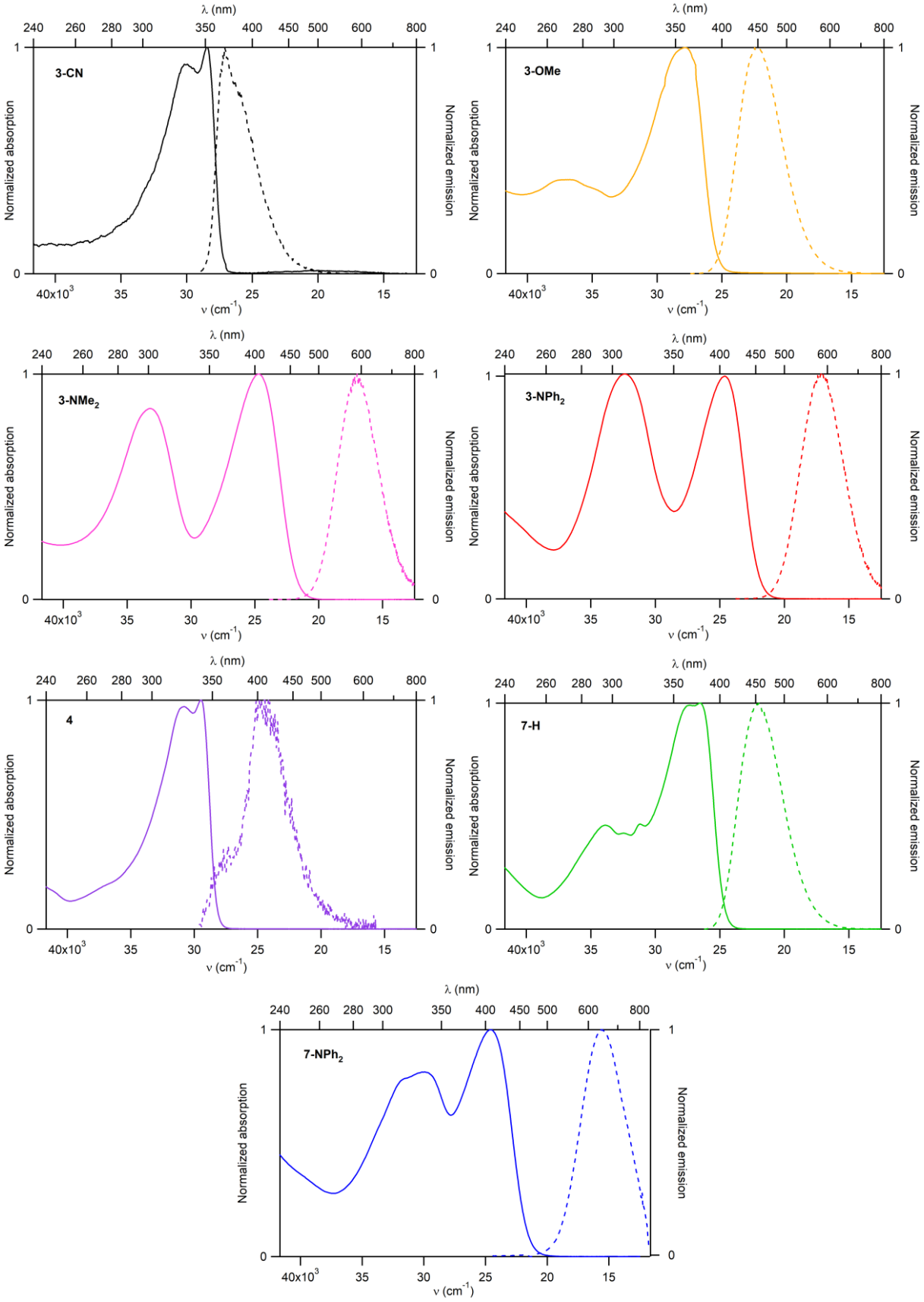


Figure S7. Normalized absorption and emission spectra in wavenumber scale (with wavelengths also shown for convenience) of compounds **3-X**, **4** and **7-X** in CH_2Cl_2 at 298K.

4. Two-photon excited fluorescence (2PEF) data for selected 3-X and 7-X derivatives

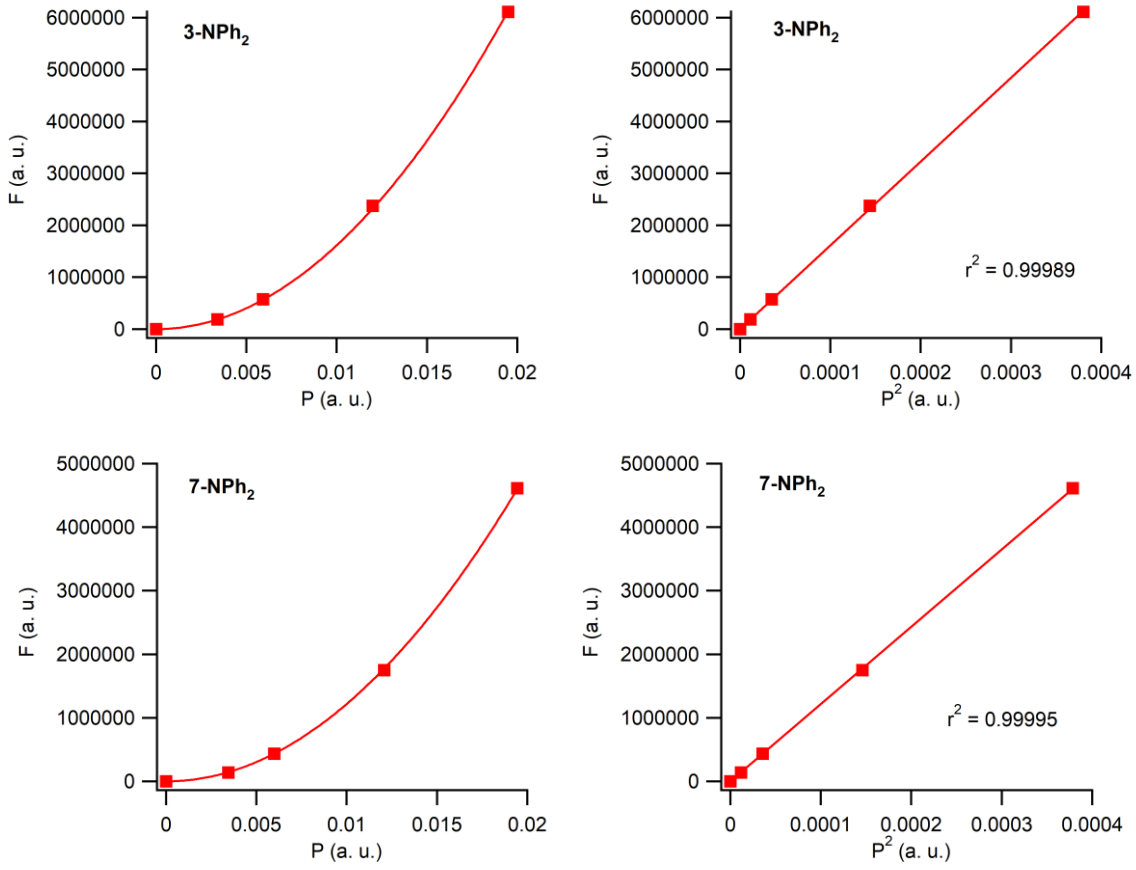


Figure S8. Left: quadratic dependence of the emission intensity (F) on laser excitation power (P) for compound **3-NPh$_2$** and **7-NPh$_2$** at 700 nm. Right: dependence of F on P^2.

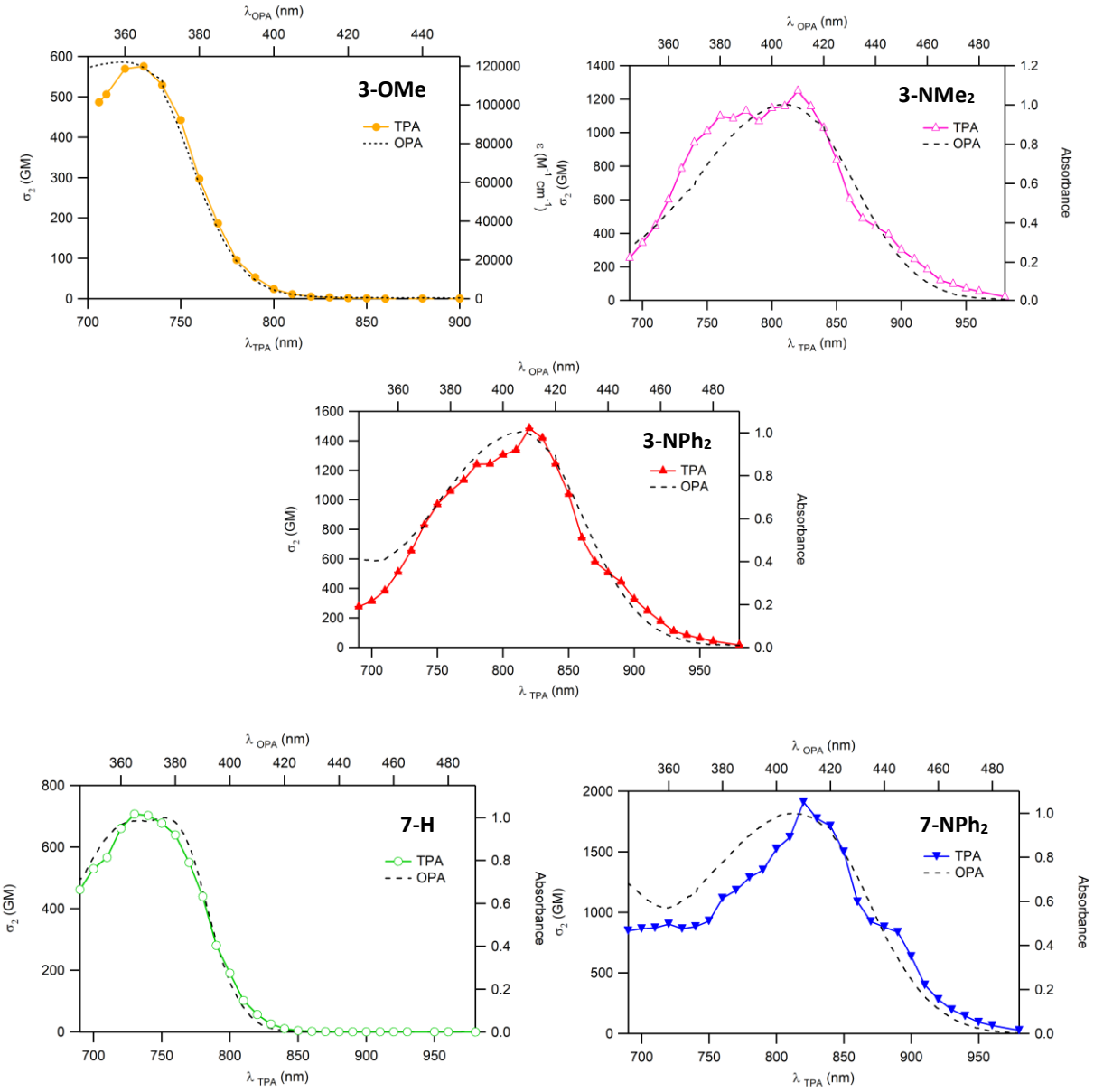
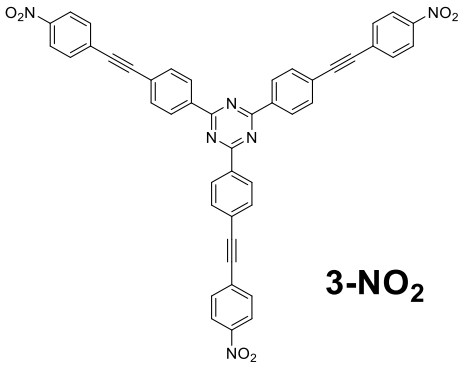


Figure S9. Overlay of one- and two-photon absorption spectra for selected **3-X** and **7-X** derivatives in CH_2Cl_2 (25 °C).

5. Cartesian coordinates of the DFT optimized geometries for 3-X, 4, 7-X and 9a-b/10a-b/11a-b



3-NO$_2$

C	1.28142352	-0.25484012	-0.00095799
N	0.43967907	-1.29259475	-0.00091999
C	-0.85999771	-0.98223076	-0.00093499
N	-1.33773650	0.26562775	-0.00075999
C	-0.41909168	1.23596480	-0.00076599
N	0.90049356	1.02590092	-0.00083899
C	-1.83366378	-2.09251811	-0.00069799
C	-3.20884532	-1.82784253	-0.00077499
C	-1.39217356	-3.42153282	-0.00044299
C	-4.12475877	-2.86575756	-0.00062499
H	-3.54791290	-0.79916528	-0.00101499
C	-2.30201198	-4.46476782	-0.00027099
H	-0.32816438	-3.62393408	-0.00043599
C	-3.68313451	-4.20073527	-0.00034999
H	-5.18835698	-2.65649630	-0.00074999
H	-1.95600240	-5.49205004	-0.00010799
C	-0.89400328	2.63421934	-0.00056899
C	0.02257007	3.69298238	-0.00069399
C	-2.26578691	2.91603093	-0.00026899
C	-0.41859407	5.00503609	-0.00055099
H	1.08298334	3.47247809	-0.00091399
C	-2.71461702	4.22550361	-0.00009399
H	-2.97283452	2.09554005	-0.00015199
C	-1.79558071	5.28975566	-0.00024699
H	0.29430957	5.82161798	-0.00065399
H	-3.77730926	4.43935488	0.00015801
C	2.72976519	-0.54276630	-0.00080199
C	3.65980259	0.50420081	-0.00099199
C	3.18823938	-1.86597493	-0.00044699
C	5.01823114	0.23800814	-0.00088999
H	3.30290303	1.52681696	-0.00124999
C	4.54506297	-2.14011261	-0.00028599
H	2.46692670	-2.67393289	-0.00028799
C	5.48026336	-1.09005946	-0.00052699
H	5.73484080	1.05134207	-0.00107199
H	4.89567654	-3.16583379	0.00000401
C	-2.25215802	6.63415330	-0.00011099
C	-2.64277127	7.78493728	0.00003601
C	6.87276895	-1.36719095	-0.00038499
C	8.06475933	-1.60392452	-0.00026799
C	-4.61943981	-5.26807742	-0.00022099
C	-5.42119993	-6.18135384	-0.00007699
C	-3.09898058	9.12839692	0.00031701
C	-2.17690626	10.19151899	0.00019001
C	-4.47787921	9.40966347	0.00061501
C	-2.61952539	11.50289266	0.00034301
H	-1.11494002	9.97729873	-0.00001399
C	-4.92591732	10.71916316	0.00086001
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C	9.91564317	-3.21076363	0.00216001
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C	12.17035408	-2.42026538	0.00063201
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H	12.47737558	-0.29564355	-0.00291500
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C	-7.73876281	-6.97948543	-0.00086099
C	-6.82352541	-9.62475169	0.00137901
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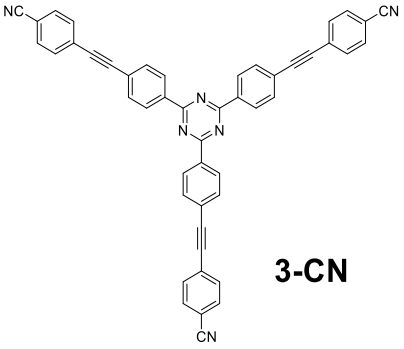

3-CN

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C	3.60661900	-0.80198100	-0.00041900
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C	4.78861800	-1.52257700	-0.00040700

H	3.62656500	0.28093200	-0.00014200
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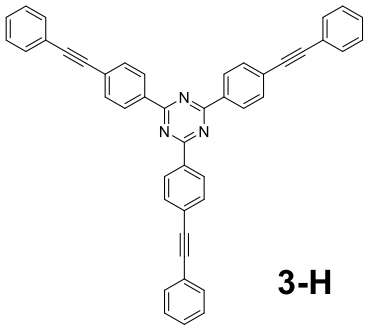

3-H

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C	-1.13797900	3.51410700	0.00011200
C	1.30759000	4.85006600	-0.00020300
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C	-1.11420200	4.89818800	0.00010200
H	-2.08253400	2.98372300	0.00023200
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H	-1.54435200	-3.29677700	0.00003900
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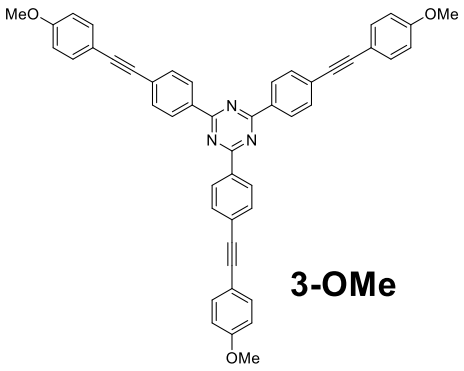

3-OMe

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C	3.79379400	-4.10495300	-0.00011000
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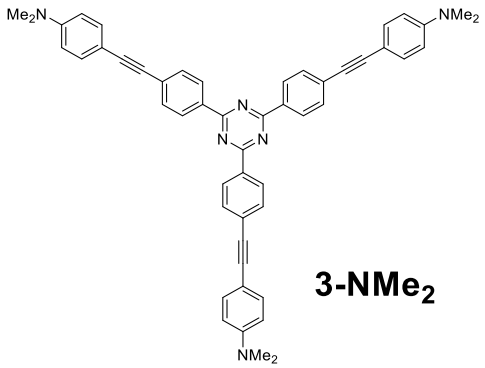

3-NMe$_2$

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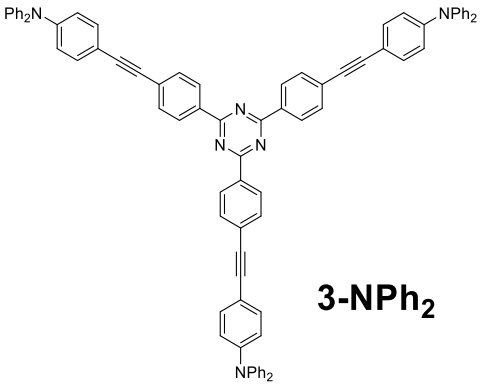

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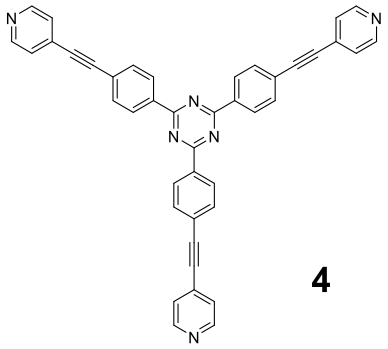

4

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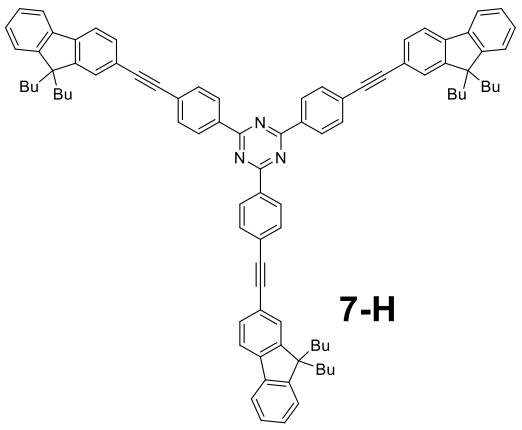

7-H

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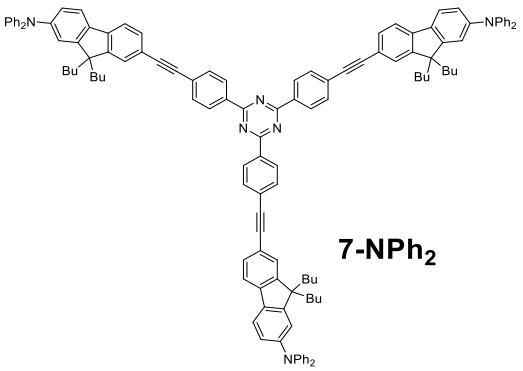

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9a

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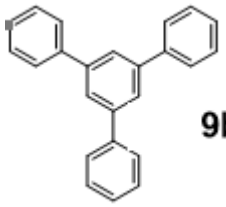

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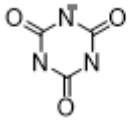

10a

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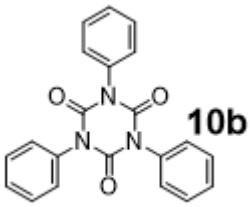

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C	0.54598200	-1.31595800	0.00023300
O	1.00974200	-2.43391900	0.00042700
C	2.77059900	-0.36291500	0.00005000
C	3.44740600	-0.45099400	1.21098100
C	3.44728100	-0.45231400	-1.21085900
C	4.82709600	-0.63191100	1.20724100
H	2.89723100	-0.37849800	2.14281200
C	4.82696500	-0.63323800	-1.20707000
H	2.89699900	-0.38081000	-2.14270300
C	5.51633900	-0.72306300	0.00010100
H	5.36232100	-0.70166000	2.14808600
H	5.36209700	-0.70402200	-2.14789000
H	6.59202600	-0.86427400	0.00011700
C	-1.07084400	2.58097900	-0.00052400
C	-1.33264000	3.21102300	-1.21159200
C	-1.33281000	3.21141300	1.21031000
C	-1.86568600	4.49636800	-1.20806700
H	-1.11992200	2.69814800	-2.14324900
C	-1.86585100	4.49675200	1.20630000
H	-1.12021600	2.69882800	2.14215600
C	-2.13212400	5.13867300	-0.00100700
H	-2.07250200	4.99480500	-2.14897700
H	-2.07280100	4.99549800	2.14701800
H	-2.54769800	6.14085500	-0.00119100
C	-1.69982100	-2.21786800	0.00047100
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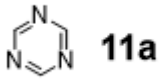
C	-2.11504900	-2.75985400	-1.21039100
C	-2.96136700	-3.86383100	1.20802400
H	-1.77738700	-2.31871800	2.14330100
C	-2.96147300	-3.86430100	-1.20632800
H	-1.77757700	-2.31954800	-2.14231000
C	-3.38432600	-4.41581100	0.00097700
H	-3.28976100	-4.29207700	2.14891000
H	-3.28995700	-4.29292400	-2.14701200
H	-4.04434000	-5.27686500	0.00117100



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H	2.05795300	-1.18976900	0.00000000
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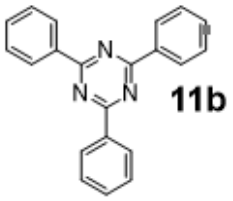

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H	-2.14058751	2.93882122	-0.00000000
C	1.20627303	4.88063538	0.00000000
H	2.14034741	2.93931201	0.00000000
C	-0.00043735	5.57841188	-0.00000000
H	-2.14805570	5.42044331	-0.00000000
H	2.14722797	5.42097799	0.00000000
H	-0.00056214	6.66370134	-0.00000000
C	2.41188695	-1.39240893	0.00000000
C	3.62808635	-0.69911557	0.00000000
C	2.42051615	-2.79233786	0.00000000
C	4.83066252	-1.39479500	0.00000000
H	3.61574405	0.38430263	0.00000000
C	3.62474264	-3.48513050	0.00000000
H	1.47647436	-3.32402447	0.00000000
C	4.83222372	-2.78869980	0.00000000
H	5.76883896	-0.84964125	0.00000000
H	3.62247628	-4.57019402	0.00000000
H	5.77229538	-3.33102768	0.00000000
C	-2.41163614	-1.39238617	-0.00000000
C	-2.42039583	-2.79230423	0.00000000
C	-3.62776909	-0.69897201	-0.00000000
C	-3.62470930	-3.48498308	-0.00000000
H	-1.47643365	-3.32411750	-0.00000000
C	-4.83040012	-1.39452434	-0.00000000
H	-3.61534914	0.38445136	-0.00000000
C	-4.83210889	-2.78844717	0.00000000
H	-3.62252666	-4.57004848	0.00000000
H	-5.76852584	-0.84928446	-0.00000000
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6. Selected frontier MOs for 3-X, 4 and 7-X

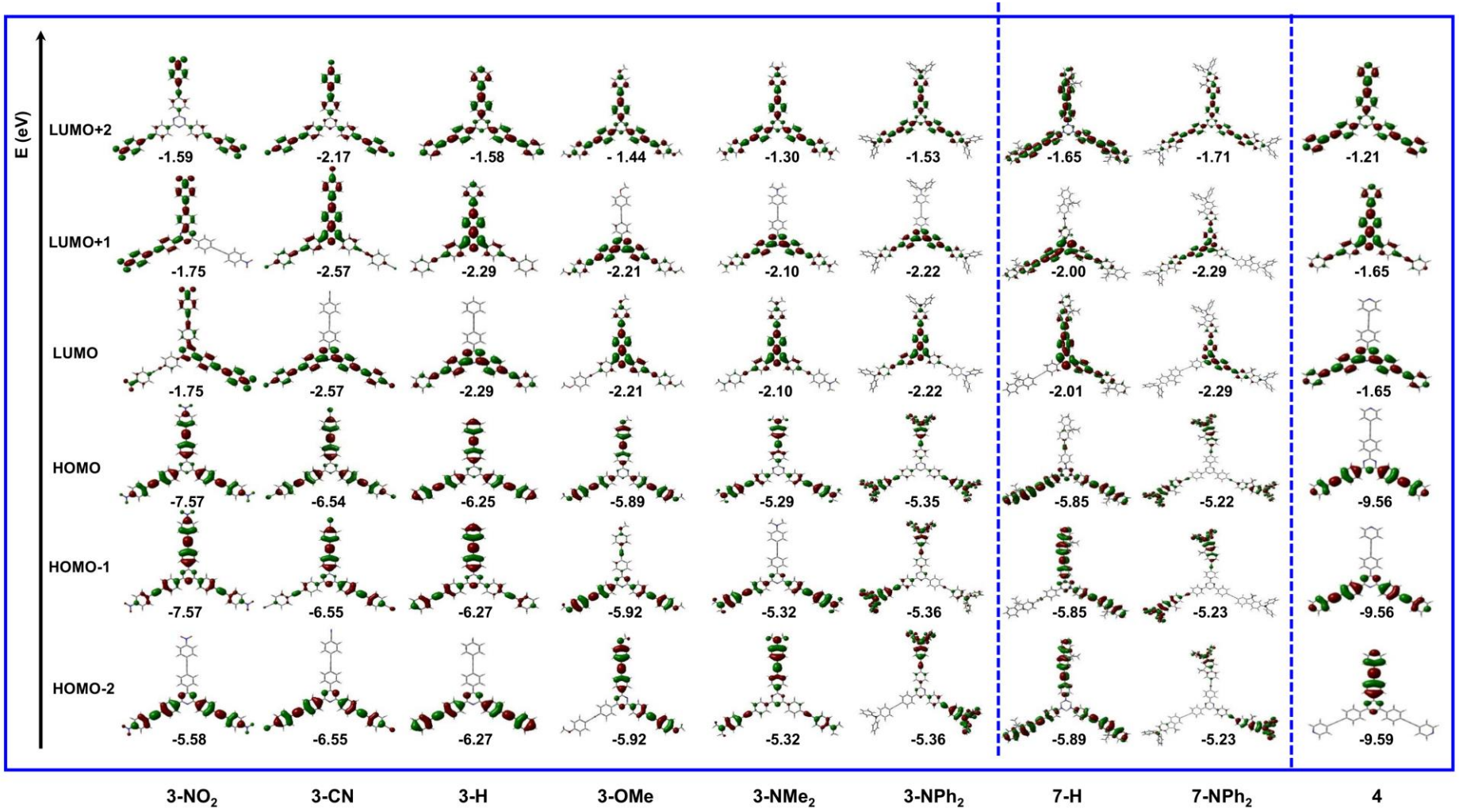
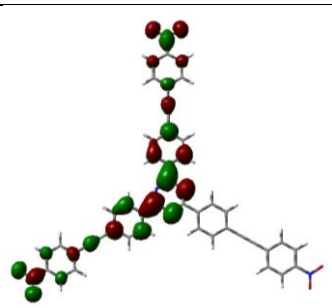
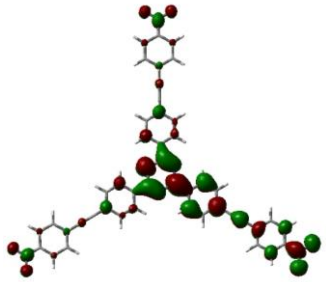
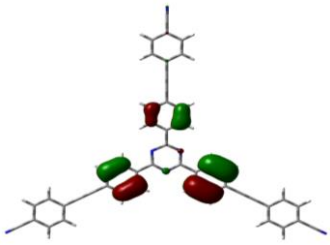
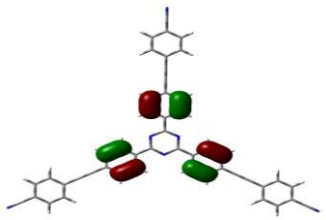
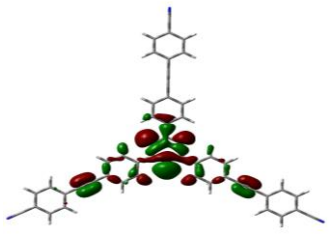
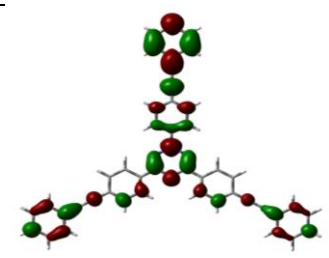
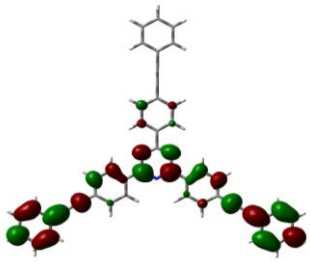
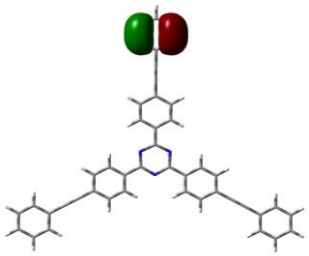
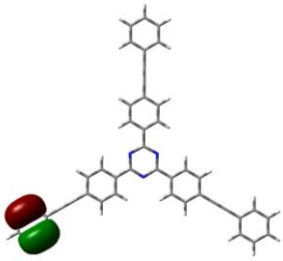
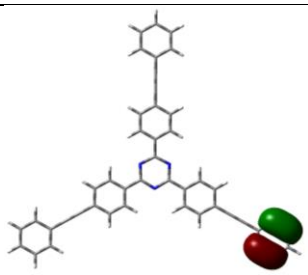
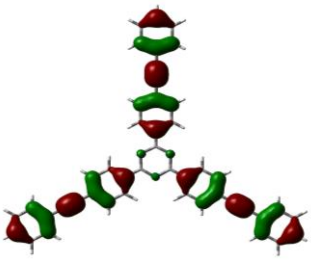
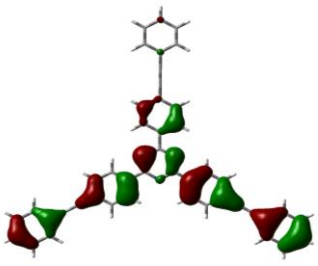
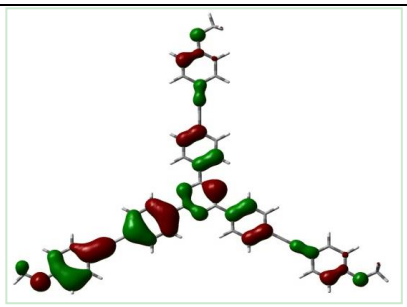
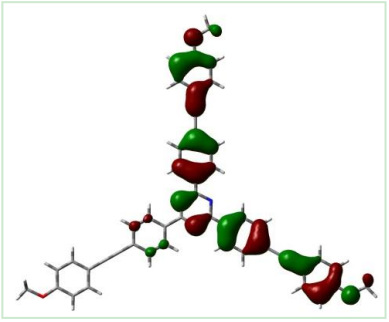
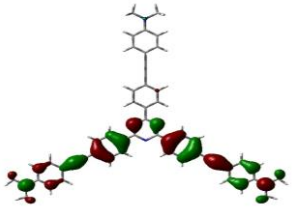
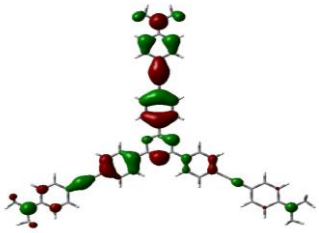
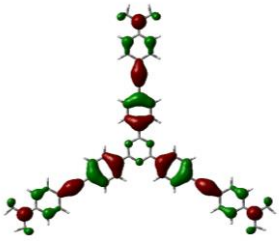
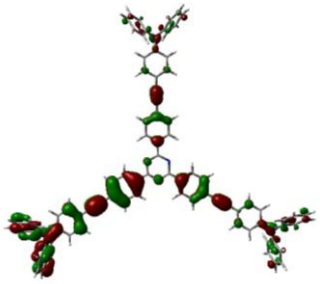
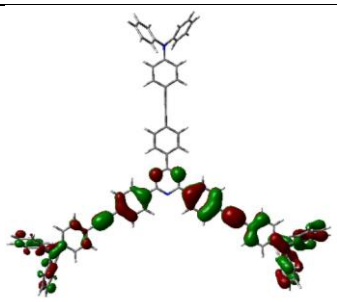
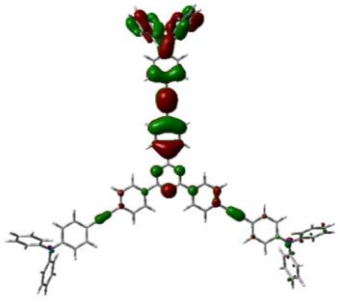
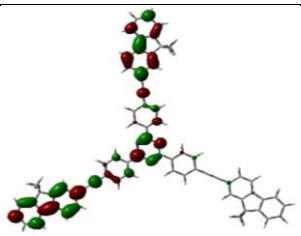
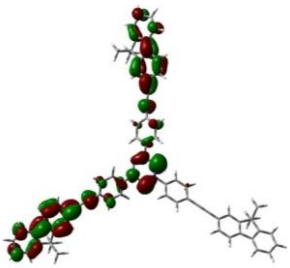
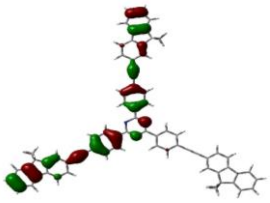
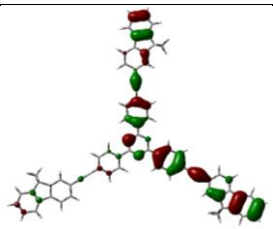


Figure S10. FMOs of **3-X**, **4** and **7-X** compounds. Contour values are ± 0.02 $(e/bohr^3)^{1/2}$.

3-NO_2	
LUMO+4	
LUMO+3	
3-CN	
HOMO-4	
HOMO-5	
HOMO-6	
3-H	
LUMO+4	

LUMO+3	
HOMO-3	
HOMO-4	
HOMO-5	
HOMO-11	
HOMO-12	
3-OMe	

HOMO-3	
HOMO-4	
3-NMe_2	
HOMO-3	
HOMO-4	
HOMO-5	
3-NPh_2	
HOMO-3	

HOMO-4	
HOMO-5	
7-H	
LUMO+4	
LUMO+3	
HOMO-3	
HOMO-4	

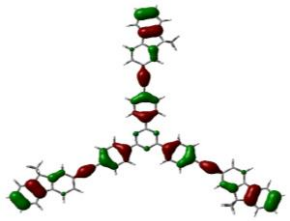
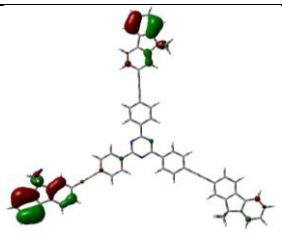
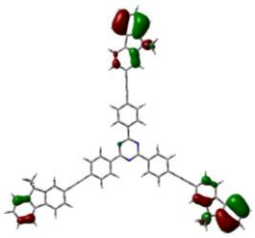
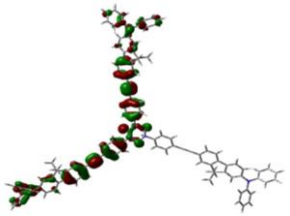
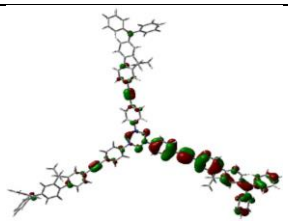
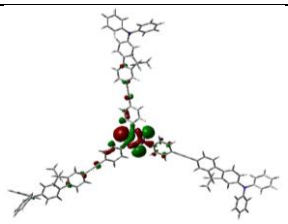
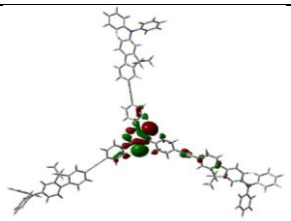
HOMO-5	
HOMO-6	
HOMO-7	
7-NPh$_2$	
HOMO-3	
HOMO-4	
HOMO-6	
HOMO-7	

Figure S11. Selected additional MOs of **3-X** and **7-X** Compounds. Contour values are ± 0.02 $(e/bohr^3)^{1/2}$.

7. Computed dipole moments for 3-X, 4 and 7-X

Table S2. Calculated (MPW1PW91/6-31G* level in CH_2Cl_2) mean deviation (°) from planarity and dipole moment (D) for for selected **3-X**, **4** and **7-X** derivatives.

Cmpd	Mean deviation from planarity (°)[a]	μ (D)
3-NO_2	0.00	0.00
3-CN	0.00	0.02
3-H	0.00	0.00
3-OMe	0.02	3.19
3- NMe_2	0.01	0.02
3-NPh_2	0.22	0.02
4	1.95	0.08
7-H	0.4	0.17
7-NPh_2	0.7	0.01

[a] Mean value of the three angles between the peripheral phenyl plane and the plane of the central core.

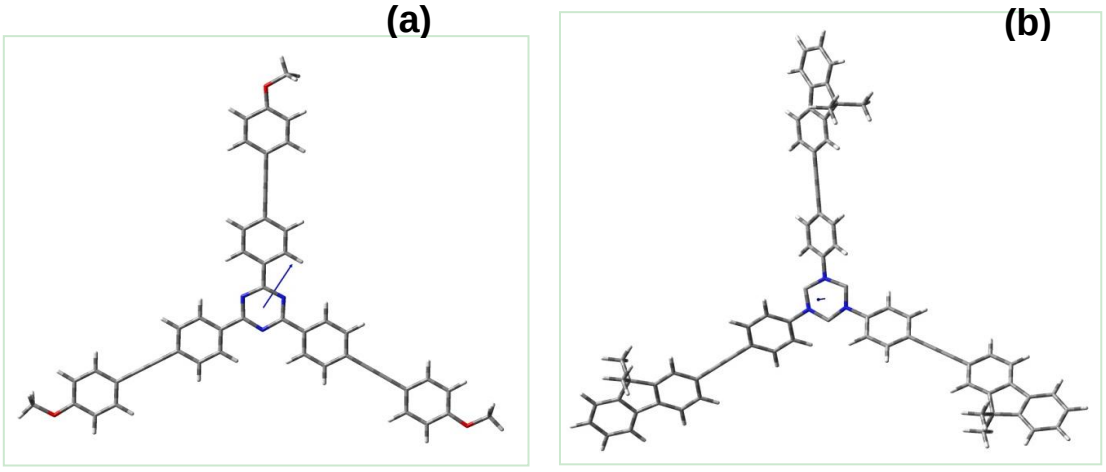


Figure S12. Dipole moments computed for **3-OMe** (a) and **7-H** (b). The main component of the dipole moment is "in" the plane of the central triazine core and results from the non-symmetric arrangement of the peripheral arms.

8. Computed bandgaps for 3-X, 4 and 7-X

Table S3. Calculated HOMO-LUMO energy gaps in CH_2Cl_2 for **3-X** (MPW1PW91 or CAM-B3LYP/6-31G* level in CH_2Cl_2).

X	HOMO-LUMO gaps (eV)	
	MPW1PW91	CAM-B3LYP
3-NO_2	3.78	5.82
CN	3.97	5.99
H	3.96	6.00
OMe	3.68	5.71
NMe_2	3.19	5.18
NPh_2	3.13	5.11

9. Computed singlet lowest-lying transitions for 3-X, 4 and 7-X

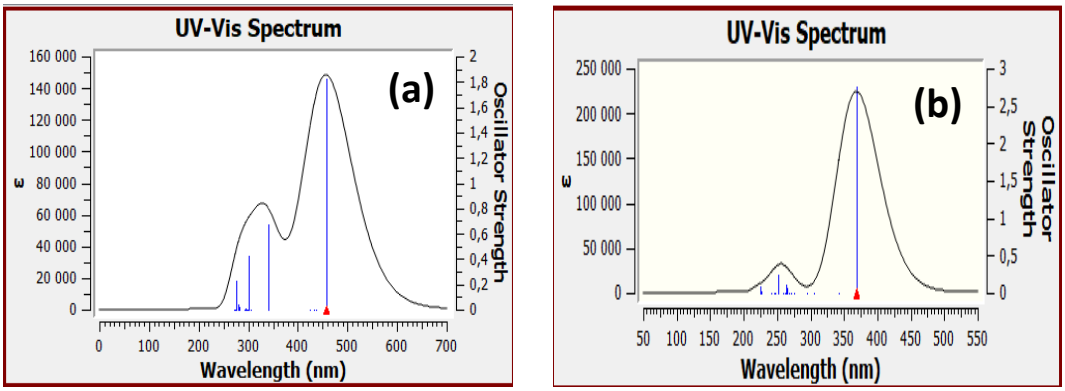


Figure S13. Computed TD-DFT (6-31G*/CH_2Cl_2) spectra for **3-NPh_2** compounds using MPW1PW91 (a) or CAM-B3LYP functionals (b).

Table S4. Nature of the relevant first computed (MPW1PW91/6-31G*) singlet excited states[a] (λ_{max} and λ_{cal} in nm, Oscillator Strength, excited state number (S_n), transition percentage and assignment) with $f \geq 0.1$ *vs.* experimental *values* in CH_2Cl_2 (PCM).

Model Cpnd [Real Cpnd]	**Experimental**	**Calculated for optimized geometry**			**Major Assignment** [f]
	λ_{max} [ε] [b]	λ_{max} [c]	λ_{cal} [*f*] [d] (S_n) [e]	Composition	
3-NO_2	377 [113]	392	392 [2.50] (S_1)	H→L (29%) H-2→L (20%) H-1→L+1 (19%) H→L+1 (13%) H-1→L+2 (11%)	$(\pi^*)_{Ph+Tri+NO2} \leftarrow (\pi)_{Ph+Tri}$
			392 [2.50] (S_2)	H→L+1 (29%) H-1→L (21%) H-2→L+1 (20%) H→L (11%) H-2→L+2 (11%)	*ibid*
		309	309 [0.13] (S_{13})	H→L+4 (40%) H-2→L+3 (15%) H-1→L+4 (14%)	$(\pi^*)_{Ph+Tri+NO2} \leftarrow (\pi)_{Ph+Tri}$
			309 [0.13] (S_{14})	H→L+3 (37%) H-1→L+3 (16%)	*ibid*
3-CN	352 [154]	374	374 [2.58] (S_1)	H→L+1 (+45%) H-2→L (+20%) H-1→L+1 (+17%)	$(\pi^*)_{Ph+Tri+CN} \leftarrow (\pi)_{Ph+Tri}$
			374 [2.59] (S_2)	H→L (35%) H-1→L (26%) H-2-→L+1 (22%)	*ibid*
	332 [sh, 142]	310	310 [0.27] (S_7)	H-1→L+2 (76%) H-1→L+2 (14%)	$(\pi^*)_{Ph+Tri+CN} \leftarrow (\pi)_{Ph+Tri}$
			310 [0.27] (S_8)	H-2→L+2 (84%)	*ibid*
3-H	/	372	372 [2.03] (S_1)	H→L+1 (49%) H-2→L (23%) H-1→L+1 (22%)	$(\pi^*)_{Ph+Tri} \leftarrow (\pi)_{Ph+Tri}$
			372 [2.03] (S_2)	H→L (47%) H-1→L (24%) H-2→L (23%)	*ibid*
	/	290	293 [0.44] (S_{11})	H-1→L+2 (93%)	$(\pi^*)_{Ph} \leftarrow (\pi)_{Ph}$
			293 [0.44] (S_{12})	H-2→L+2 (93%)	*ibid*
			255 [0.17] (S_{30})	H-11→L+1 (25%) H-12→L (25%) H→L+4 (15%) H-13→L+1 (13%)	$(\pi^*) \leftarrow (\pi)$
3-OMe	359 [122]	398	398 [2.04] (S_1)	H→L+1 (52%) H-2→L (12%) H-1→L+1 (11%) H-1->→L (11%) H-2→L+1 (10%)	$(\pi^*)_{Ph+Tri} \leftarrow (\pi)_{Ph+Tri+OMe}$
			398 [1.95] (S_2)	H→L (49%) H-1→L (12%) H-2→L (12%) H-2→L+1 (12%) H-1→L+1 (11%)	*ibid*

			382 [0.00] (S_3)	H-1→L+2 (48%) H-2→L+1 (46%)	*Ibid* [g]
	270 [51]	300	306 [0.44] (S_7)	H-1→L+2 (93%)	$(\pi^*)_{Ph+OMe} \leftarrow (\pi)_{Ph+OMe}$
			306 [0.44] (S_8)	H-2→L+2 (92%)	*ibid*
			274 [0.22] (S_{18})	H-3→L+1 (20%) H-4→L (19%) H-5→L+1 (18%) H-4→L+1 (11%) H-3→L (10%)	$(\pi^*) \leftarrow (\pi)$
3-NMe$_2$	405 [105]	457	457 [1.82] (S_1)	H→L (47%) H-1→L+1 (20%) H-2→L (12%)	$(\pi^*)_{Ph+Tri} \leftarrow (\pi)_{Ph+Tri+NMe2}$
			457 [1.82] (S_2)	H→L+1 (34%) H-1→L (13%) H-2→L+1 (13%)	*ibid*
	301 [89]	340	340 [0.67] (S_7)	H-1→L+2 (89%)	$(\pi^*)_{Ph+OMe} \leftarrow (\pi)_{Ph+NMe2}$
			340 [0.67] (S_8)	H-2→L+2 (89%)	*ibid*
			301 [0.22] (S_{18})	H-5→L (22%) H-3→L+1 (17%) H-4→L (17%) H-3→L (12%) H-4→L+1 (12%) H-5→L+1 (10%)	$(\pi^*) \leftarrow (\pi)$
3-NPh$_2$	406 [99]	465	465 [1.83] (S_1)	H→L (31%) H→L+1 (20%) H-2→L (19%) H-1→L+1 (18%)	$(\pi^*)_{Ph+Tri} \leftarrow (\pi)_{Ph+NPh2}$
			465 [1.83] (S_2)	H→L+1 (30%) H-1→L (20%) H-2→L+1 (19%) H→L (19%)	*ibid*
	309 [100]	340	359 [0.72] (S_7)	H-1→L+2 (84%)	$(\pi^*)_{Ph+OMe} \leftarrow (\pi)_{Ph+NMe2}$
			359 [0.72] (S_8)	H-2→L+2 (85%)	*ibid*
			330 [0.57] (S_{11})	H-4→L+1 (29%) H-5→L+2 (27%) H-3→L+1 (13%) H-3→L (10%) H-4→L (9%)	$(\pi^*) \leftarrow (\pi)$
4	339 [112]	356	356 [2.15] (S_1)	H→L (70%) H-1→L (24%)	$(\pi^*)_{Py+Tri} \leftarrow (\pi)_{Py+Tri}$
			354 [2.13] (S_2)	H-2→L+1 (57%) H-1→L (29%)	*ibid*
	270 [sh, 21]	289	289 [0.33] (S_{11})	H-1→L+2 (91%)	$(\pi^*) \leftarrow (\pi)$
			289 [0.26] (S_{12})	H→L+2 (71%) H-2→L+2 (20%)	*ibid*
7-H	377 [173]	410	410 [2.5] (S_1)	H→L+1 (49%) H-1→L (16%) H-2→L+1 (15%)	$(\pi^*)_{Flu+Tri} \leftarrow (n)_{Flu}$
			410 [2.5] (S_2)	H→L (+47%) H-2→L (17%) H-1→L+1 (16%)	*ibid*
	321 [67]	325	325 [0.62] (S_8)	H-1→L+2 (88%)	$(\pi^*)_{Flu+Tri} \leftarrow (\pi)_{Flu}$

			325 [0.62] (S_9)	H-2→L+2 (88%)	*ibid*
	295 [66]	296	296 [0.18] (S_{15})	H-5→L+1 (30%) H-4→L+1 (23%) H-3→L (21%)	$(\pi^*)_{Flu+} \leftarrow (\pi)_{Flu}$
			296 [0.18] (S_{16})	H-5→L (32%) H-3→L+1 (22%) H-4→L (21%)	*ibid*
7-NPh$_2$	406 [129]	483	483 [1.72] (S_1)	H→L+1 (50%) H-1→L (17%) H-2→L+1 (11%)	$(\pi^*)_{Flu+Tri} \leftarrow (\pi)_{Flu+NPh2}$
			483 [1.72] (S_2)	H→L (38%) H-2→L (16%) H-1→L+1 (16%)	*ibid*
	334 [105]	388	388 [1.20] (S_7)	H-1→L+2 (72%)	$(\pi^*)_{Flu} \leftarrow (\pi)_{Flu+NPh2}$
			388 [1.20] (S_8)	H-2→L+2 (71%)	*ibid*
	317 [sh, 101]		369 [0.63] (S_{10})	H-3→L+1 (35%) H-5→L (19%) H-4→L+1 (18%)	$(\pi^*)_{Flu} \leftarrow (\pi)_{Flu+NPh2}$
			369 [0.63] (S_{11})	H-3→L (33%) H-4→L (21%) H-5→L+1 (19%)	*ibid*

[a] excited states calculated after optimisation are all ^{1}A. [b] Experimental absorption (nm) and extinction coefficients (ε) in 10^3 $M^{-1}.cm^{-1}$. [c] λ_{max} and λ_{cal} are the maximum wavelength obtained from the simulated absorption bands, and the TD-DFT calculated wavelength of a singlet excitation, respectively in nm. [d] Computed oscillator strength. [e] Excited state number. [f] Tri: s-triazine core, Flu: fluorene core, Ph/Py: phenyl or pyridyl rings. [e] Forbidden transition (A symmetry) corresponding S_1 and S_2 (*E* symmetry set in strict D_3 symmetry).

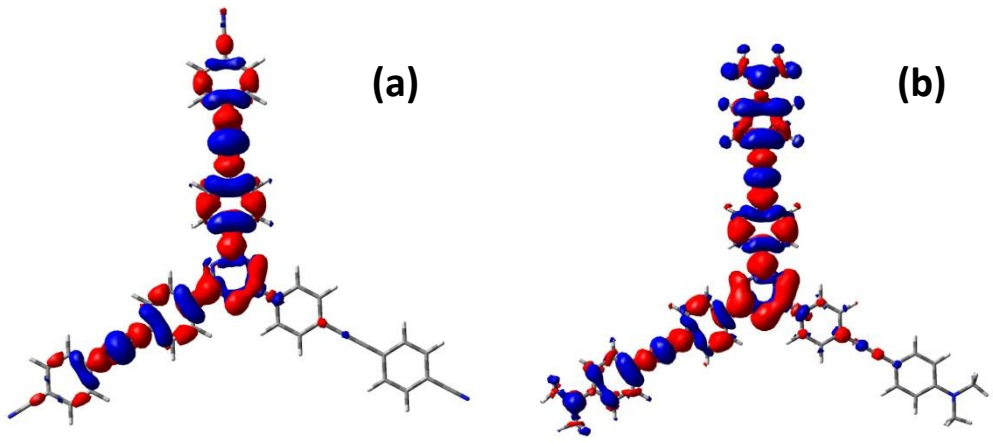


Figure S14. Density difference plots ($\Delta\rho(r)= \rho_{S1}(r)- \rho_{S0}(r)$) computed for **3-CN** (a) and **3-NMe$_2$** (b) between S_1 and S_0 states (red = increase, blue = decrease of electron density; isovalue 0.02 au).

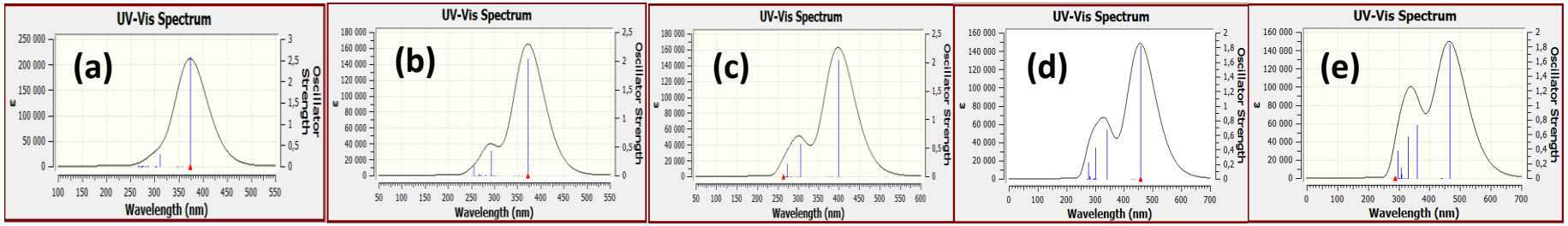


Figure S15. Computed TD-DFT spectra (MPW1PW91/6-31G*/CH_2Cl_2) for **3-X** compounds; X = CN (a), H (b), OMe (c), NMe_2 (d) and NPh_2 (e).

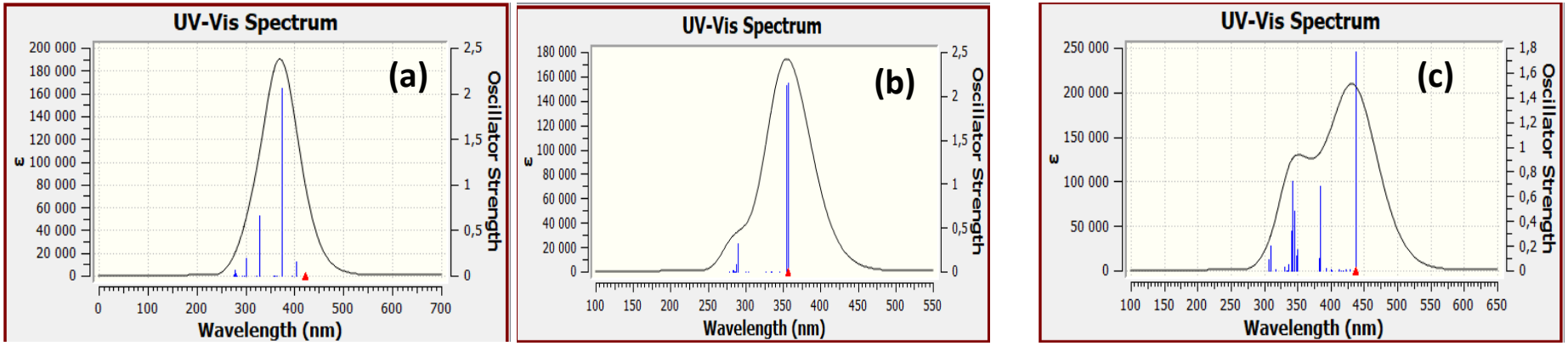


Figure S16. Computed TD-DFT spectra (MPW1PW91/6-31G*/CH_2Cl_2) for **7-X** compounds (X = H (a) and NPh_2 (b) and **4** (c).

10. Computed 2PA spectra for selected 3-X and 7-X compounds

Method used to derive the 2PA cross-sections:

The 2PA cross-section σ^{TPA} has been obtained from the imaginary part of the third-order hyperpolarizability γ using the following expressions: [1,2]

$$\sigma^{TPA} = \frac{N\pi^3\alpha^2\hbar^3\omega^2}{15e^4}\gamma^{TPA} \quad (1)$$

$$\gamma^{TPA} = \sum_{\alpha\beta}(\mathrm{Im}\gamma_{\alpha\alpha\beta\beta} + \mathrm{Im}\gamma_{\alpha\beta\beta\alpha} + \mathrm{Im}\gamma_{\alpha\beta\alpha\beta}) \quad (2)$$

Where α is the fine structure constant (not to be confused with the α index of the summation in eq 2), e is the elementary charge, ω is the photon energy, $\hbar$ is the reduced Planck's constant whereas the integer value $N = 4$ is used for all simulated TPA spectra.[2]

The σ^{TPA} value is usually given in Göppert-Mayer units (1 GM = 10^{-50} cm^4 s photon^{-1}).[3]

We first evaluate σ^{TPA} in atomic units and then multiply it by (0.529177 × 10^{-8} cm/a.u.)^4 × (2.418884 × 10^{-17} s/a.u.) to obtain its value in the conventional units (cm^4 s photon^{-1}).

[1] Silverstein, D. W.; Jensen, L. *J. Chem. Phys.* (2012) *136*:064111.
[2] Beerepoot, M. T. P.; Friese, D. H.; List, N. H. Kongsted, J.; Ruuda, K. *Phys. Chem. Chem. Phys.* **2015**, *17*, 19306-19314.
[3] Göppert-Mayer, M. *Ann Phys (Leipzig)* **1931,** *9*,273-294.

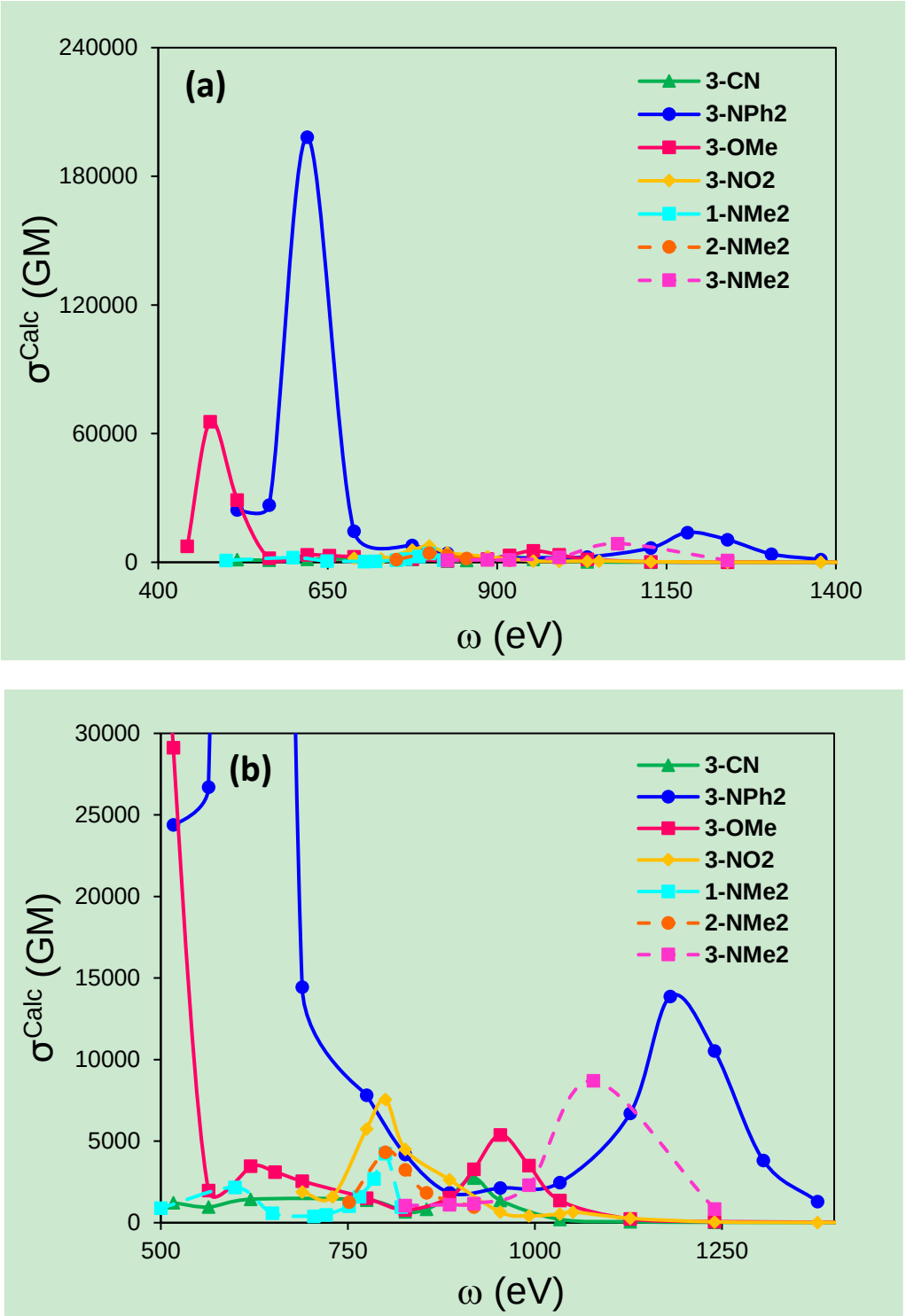


Figure S17. (a) Theoretical TPA profiles for selected **3-X** and **7-X** compounds computed at the SAOP/DZP level. (b) Detailled view.

Table S5. Computed energies and cross-sections for 2PA maxima at the SAOP/DZP level.

Cpnd	2PA	
	ω (eV)	σ^{TPA} (GM)
3-NO_2	1.18	660
	1.55	7560
3-CN	1.35	2735
	2	1440
3-OMe	1.3	5391
	2.6	65605
3-NPh_2	1.05	13875
	2	198231
7-H	1.2	7260
	1.45	3323
7- NPh_2	0.9	21531
	1.4	9074

11. Derivation of N_{eff} values for 1-X, 2-X, 3-X, 4, 7-X and 7-X derivatives

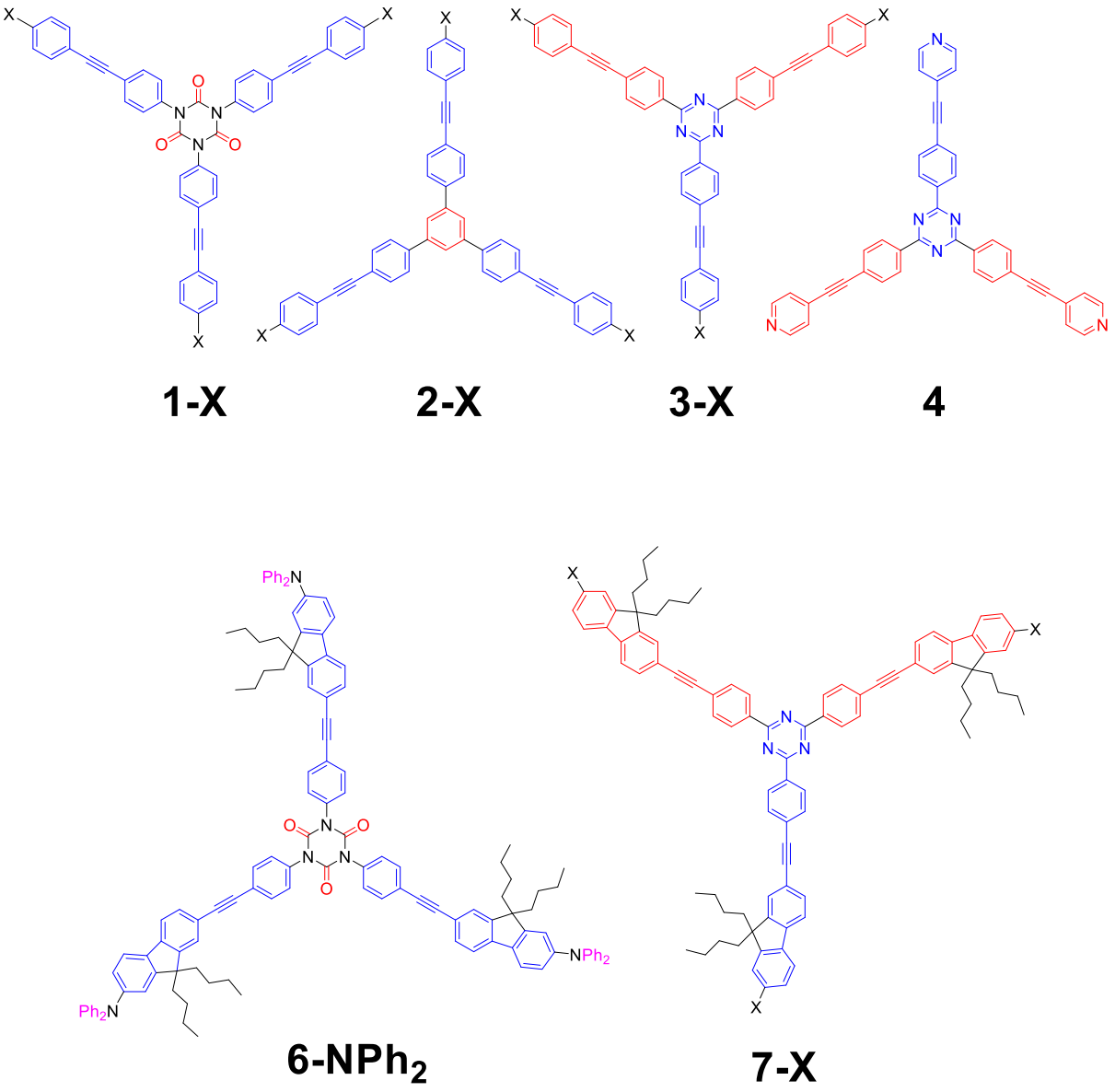


Figure S18. The independant π-manifolds (containing each N_i π-electrons) which were considered in the various compounds for the calculation of N_{eff} (using the formula: $(N_{eff})^2 = \Sigma_i(N_i)^2$) are set in different colors. These were chosen based on conformational and topological issues. For X = CN, the N_i value for the attenant π-manifold was incremented of two units) and for X = NPh_2, two additional π-manifold of 6 electrons each were considered).

12. References

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